Large Broadening of the Superconducting Transition by Fluctuations in a 3D Metal at High Magnetic Fields: The MgB_2 case.

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It is shown that the transition to the low temperature superconducting state in a 3D metal at high magnetic field is smeared dramatically by thermal fluctuation of the superconducting order parameter. The resulting superconducting-to-normal crossover occurs in a vortex liquid state which is extended well below the mean-field H_{c2}. Application to MgB_2 yields good quantitative agreement with recently reported data of dHvA oscillation in the superconducting state.

It is well known that the transition from the normal to the superconducting (SC) state in type-II 3D superconductors in the absence of external magnetic field is a sharp, second-order phase transition, with a vanishing order parameter at the transition temperature T_c continuously growing with the decreasing temperature below T_c. Fluctuations effect can smear the transition significantly in high T_c and low-dimensional superconductors [1], where the phase space accessible for the fluctuations is dramatically enhanced. The influence of an external magnetic field is similar to an effective reduction of dimensionality[2], resulting in a significant smearing of the transition even at very low temperatures. Such strong smearing effects have been observed in varies quasi 2D low T_c superconductors at high magnetic fields [3],[4],[5].

In the present paper we show theoretically, and confirm by comparison with very recent de-Haas van-Alphen (dHvA) oscillation data in the SC state [6], that the smearing of the SC transition by fluctuations in a conventional 3D type-II superconductor, such as MgB_2, at high magnetic fields, is surprisingly strong, comparable in magnitude to that in 2D superconductors. This conclusion is reached by generalizing the Bragg-chain model of the 2D vortex liquid state at high perpendicular magnetic field[7] to an array of strongly coupled 2D SC layers. Within this model it is found that, similar to the situation in a single 2D SC layer, the vortex lattice melting point in a 3D superconductor at low temperature T is located well below the mean-field (MF) upper critical field $H_{c2}(T)$, so that in a broad field range above the melting point the corresponding system of fluctuations is equivalent to a 1D array of SC quantum dots at zero magnetic field [8].

Our starting point is the microscopic BCS Hamiltonian for electrons in a layered 3D metal, interacting via an effective two-body attractive potential, under the influence of a strong static magnetic field. We assume, for simplicity, that the magnetic field direction (along z-axis) is perpendicular to the layers situated in (x, y)-plane. Writing down the functional integral expression for the partition function of this system, the electronic field can be eliminated by introducing bosonic complex field $\Delta(\mathbf{r})$ (by means of the Hubbard-Stratonovich transformations), which describes all possible realizations of Cooper-pairs condensates [9],[7]. Expansion of the resulting free energy functional, $F_G[\Delta(\mathbf{r})]$, in the order parameter up to the quartic term is a good approximation for magnetic fields around mean field H_{c2}.

In the lowest Landau level approximation, which is valid at high magnetic fields and low temperatures [10], the most general form of the order parameter $\Delta(\mathbf{r})$ is a coherent superposition of Landau wave functions, $\phi_q(x, y) = \exp\left[iqx - (y/a_H + qa_H/2)^2\right]$:

$$\Delta(x, y, z) = \sum_{n,m} c_q(z)\, \phi_q(x, y) \qquad (1)$$

where $c_q(z)$ are arbitrary complex functions of the coordinate z , defined on the quasi continuous lattice $q = \frac{2\pi}{a_x a_H}\left(n + m/\sqrt{N}\right)$, $n, m = -\sqrt{N}/2 + 1, \ldots, \sqrt{N}/2$, which determines the projections of the orbital guiding centers on the y axis. Here N is the total number of flux lines threading the SC sample, and $a_H = \sqrt{c\hbar/eH}$ is the magnetic length. In the case when all the coefficients c_q are different from zero there is one to one correspondence between all N guiding centers and their projections on the y axis.

As discussed in detail in Ref.[11], such a quasi continuous configuration costs a large fraction of the total SC condensation energy, and may be therefore omitted at magnetic fields well below MF H_{c2}. In this region it is sufficient to use in Eq.(1) a discrete subset of $\sqrt{N}$ Landau orbitals $\phi_{q_n}(x, y)$, with $q_n = \frac{2\pi}{a_x a_H} n$, $n = 0, \pm 1, \pm 2, \ldots$. Including the omitted high energy modes would always increase the fluctuation effect. Thus, near and above the MF transition the fluctuation effect, calculated in the discrete chain approximation, should always underestimate the observed effect. On the other hand, an upper bound on the fluctuation effect can be obtained from the 2D model [13], where the discrete chain representation yields reasonably good agreement with exact numerical simulation [14].

Writing $c_{q_n}(z) \equiv c_n(z) = |c_n(z)|\, e^{i\varphi_n(z)}$ the phase $\varphi_n(z)$ determines the relative lateral position $x_n = -\varphi_n/q_n$ of the n-th Landau orbital within a single 2D

layer. It can be readily shown that, by selecting the x axis along the principal crystallographic axis of the 2D Abrikosov vortex lattice, the variables $\xi_n \equiv \varphi_n - \varphi_{n-1}$ describe the lateral positions of the most easily sliding vortex chains in the vortex lattice, which are generated mainly by interference between two neighboring Landau orbitals [11].

The corresponding free energy functional, projected on the subspace of the lowest Landau level, can be written in a local anisotropic Ginzburg-Landau (GL) form [7],[12]:

$$F_{GL} = \int \frac{d^3r}{\upsilon}\left[-\alpha\left|\Delta\left(\mathbf{r}\right)\right|^2 + \frac{\beta}{2}\left|\Delta\left(\mathbf{r}\right)\right|^4 + \gamma\left|\frac{\partial\Delta\left(\mathbf{r}\right)}{\partial z}\right|^2\right] \tag{2}$$

where $\upsilon = \pi a_H^2 d$ is the volume of a single vortex per layer and the effective GL coefficients α,β, and γ, can be expressed in terms of the microscopic normal electron parameters (see below). It is convenient to divide the length L_z of the sample perpendicular to the layers into N_z segments of length d , $L_z = N_z d$, where d is the interlayer distance, and define a discrete set $c_{n,\zeta} = |c_{n,\zeta}|\, e^{i\varphi_{n,\zeta}} \equiv c_n\left(z_\zeta\right)$, $\zeta = 1, 2, ...N_z$, with the periodic boundary conditions: $c_{n,N_z+1} = c_{n,1}$.

Using Eq.(1) the partition function,

$$\mathcal{Z} \equiv \mathcal{Z}_{ch}^{\sqrt{N}} = \int D\Delta\left(\mathbf{r}\right) D\Delta^{\star}\left(\mathbf{r}\right) \exp\left\{-F_{GL}\left[\Delta\left(\mathbf{r}\right)\right]/k_BT\right\}$$

where $\mathcal{Z}_{ch}$ is evaluated as a multiple integral: $\prod_{n,\zeta}\int|c_{n,\zeta}|d|c_{n,\zeta}|\int d\varphi_{n,\zeta}e^{-F_{GL}/(\sqrt{N}k_BT)}$, with

$$\begin{aligned}\frac{F_{GL}}{\left(a_x/\sqrt{2\pi}\right)\sqrt{N}} &= -\alpha\sum_{n,\zeta}\left|c_{n,\zeta}\right|^2 + \eta\sum_{n,\zeta}\left|c_{n,\zeta+1} - c_{n,\zeta}\right|^2 \\ &+ \frac{\beta}{2^{3/2}}\sum_{n,s,p;\zeta}\lambda^{s^2+p^2}|c_{n,\zeta}||c_{n+s+p,\zeta}||c_{n+s,\zeta}||c_{n+p,\zeta}| \\ &\times e^{i\left(\varphi_{n+s,\zeta}+\varphi_{n+p,\zeta}-\varphi_{n,\zeta}-\varphi_{n+s+p,\zeta}\right)}\end{aligned} \tag{3}$$

and $\eta = d^2\gamma$. In this Landau orbital representation of the GL functional, Eq.(2), the off-diagonal elements constitute a rapidly convergent series in the small expansion parameter $\lambda \equiv e^{-(\pi/a_x)^2} \approx 0.066$, where all terms of order higher than the second may be neglected.

For the 3D electronic band structure under study here the characteristic interlayer Josephson tunneling amplitude η is much larger than the minimal intra-layer shear stiffness, $4\lambda^2 \sim 10^{-2}$, characterizing the principal axis, x, in the vortex lattice. Under this condition the low energy fluctuations of $\Delta\left(\mathbf{r}\right)$ correspond to collectively sliding chains of vortices in different layers, such that the corresponding fluctuating magnetic flux lines remain nearly parallel to each other (and so to the external magnetic field). Similar to the situation in a 2D superconductor [7], these low-lying shear fluctuations determine the vortex lattice melting point to be well below H_{c2}.

For magnetic fields H above this melting point the second order terms in λ, which oscillate as functions of the phases $\varphi_{n,\zeta}$, are averaged to zero by the integrations over $\varphi_{n,\zeta}$, and the effective free energy functional F_{GL} can be written in the very simple, independent vortex chain form $F_{GL} = \sqrt{N}\sum_n f_{GL}^n$, with

$$\begin{aligned} f_{GL}^n &= \frac{a_x}{\sqrt{2\pi}}\sum_{\zeta}\left\{-\alpha\left|c_{n,\zeta}\right|^2 + \frac{\beta}{2^{3/2}}\left|c_{n,\zeta}\right|^4\right. \\ &+ \left.\eta\left|c_{n,\zeta+1} - c_{n,\zeta}\right|^2\right\},\end{aligned} \tag{4}$$

which may be considered as an effective GL energy functional for a single vortex line. In this expression we have also neglected the first order terms in λ, since they effectively yield a small additive correction to β, so that their influence on the critical behavior is unimportant [13].

The calculation of the corresponding partition function is rather straightforward. The phase variables, $\varphi_{n,\zeta}$, can be readily integrated out. The resulting expression can be written as a functional integral over the squared amplitude $y_\zeta \equiv \left(\beta a_x/2k_BT\sqrt{\pi}\right)^{1/2}\left|c_\zeta\right|^2$, with an effective GL functional, incorporating phase fluctuations:

$$\begin{aligned} f_{GL,eff} &= k_BT\sum_{\zeta}\Big(-\sqrt{2}xy_\zeta + \frac{1}{2}y_\zeta^2 + 2\kappa y_\zeta \\ &- \ln I_0\left(2\kappa\sqrt{y_\zeta y_{\zeta+1}}\right)\Big)\end{aligned} \tag{5}$$

$$x \equiv \frac{\alpha}{\sqrt{2\beta\beta_a k_BT}} \quad ; \qquad \kappa \equiv \frac{\eta}{\sqrt{\beta\beta_a k_BT}}; \qquad \beta_a \equiv \frac{\sqrt{\pi}}{a_x}$$

Here and below, for the sake of notation simplicity, we drop the vortex chain indices.

We can then estimate the partition function in two limiting situations, for weak ($\kappa \ll 1$) and strong ($\kappa \gg 1$) interlayer coupling. In the former limit the integrals over amplitudes can be calculated explicitly with the well known result [7],[13]. It is convenient to define the partition function per single vortex per layer, $\mathcal{Z}_v \equiv \mathcal{Z}^{1/\mathcal{N}}$ ($\mathcal{N} = NN_z$), which is given by:

$$\ln\frac{\mathcal{Z}_v}{\mathcal{Z}_0} = x^2 + \ln \operatorname{erfc}\left(-x\right) \tag{6}$$

where $\operatorname{erfc}(x) \equiv \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-y^2}dy$. For strong interlayer coupling the result is obtained by using the steepest descend integration, leading to

$$\begin{aligned}\ln\frac{\mathcal{Z}_v}{\mathcal{Z}_0'} &= \sqrt{2}xy_0 - \frac{1}{2}y_0^2 - \frac{1}{2}\ln\left(4\pi\kappa\right) \\ &- \ln\frac{\left(x^2+1\right)^{1/4} + \sqrt{\left(x^2+1\right)^{1/2} + 2^{1/2}\kappa}}{2^{3/4}}\end{aligned} \tag{7}$$

where $y_0 = \left(x + \sqrt{x^2+1}\right)/\sqrt{2}$. In Eqs.(6,7) $\mathcal{Z}_0$ and $\mathcal{Z}_0'$ are constants (i.e. independent of both x and κ), and so are thermodynamically unimportant.

Thus, in the liquid state above the vortex lattice melting point one can readily derive simple limiting expressions for the spatially averaged mean square order parameter, $\left\langle\overline{|\Delta|^2}\right\rangle \equiv \int d^3r\left\langle\left|\Delta\left(\overrightarrow{r}\right)\right|^2\right\rangle/\left(\mathcal{N}\upsilon\right)$, in the general

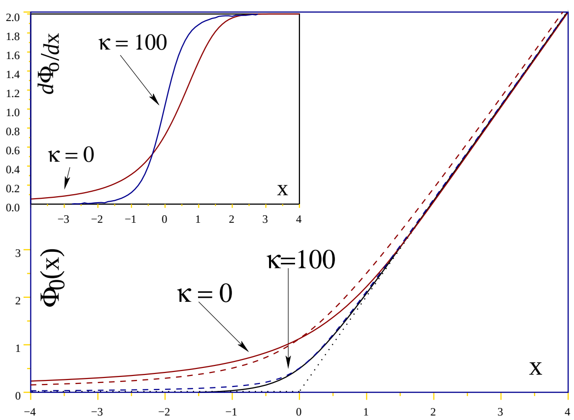

FIG. 1: The spatially averaged mean-squared order parameter, measured in units of α_{0I} , as a function of the scaling parameter $x = \alpha/\sqrt{2\beta\beta_a k_B T}$ (see text) around the mean-field transition point $x = 0$ in the weak and strong coupling limits (Solid lines). Dashed lines represent the corresponding results calculated from a simple interpolation formula. The doted straight line represents the result of mean-field theory. Inset: The derivative with respect to x is plotted to emphasize the crossover region.

from:

$$\left\langle \overline{|\Delta|^2} \right\rangle = \frac{k_B T}{\mathcal{N}} \frac{\partial \ln \mathcal{Z}}{\partial \alpha} = \sqrt{\frac{k_B T}{2\beta\beta_a}} \left(\frac{\partial \ln \mathcal{Z}_v}{\partial x} \right) \equiv \alpha_{0I} \Phi_0(x;\kappa) \tag{8}$$

where $\alpha_{0I} = \sqrt{\frac{k_B T}{2\beta\beta_a}}$. The function $\Phi_0(x;\kappa) \equiv \frac{\partial \ln \mathcal{Z}_v}{\partial x}$ for $\kappa = 0$ and $\kappa = 100$ is shown in Fig. (1). With increasing interlayer coupling the mean-square order parameter at the MF transition point decreases rapidly within the small interval $0 \leq \kappa \leq 1$, then saturating at a non-vanishing value in the entire strong coupling region $\kappa > 1$.

The non-vanishing value of $\left\langle \overline{|\Delta|^2} \right\rangle$ at the MF transition point reflects smearing of the phase transition to the SC state due to fluctuations. This effect characterizes the GL theory of a 3D superconductor at high magnetic fields, since above the vortex lattice melting point it can be mapped to the GL theory of a 1D superconductor at zero magnetic field, where a genuine phase transition is absent[15]. In the zero coupling limit, $\eta \to 0$, the effective GL free energy functional in a given SC layer, appearing within the curly brackets in Eq.(4), is equivalent to the GL energy functional for a 0D superconductor near the SC transition at vanishing magnetic field [8]:

$$f_{GL}^{(0)}\left(|\psi|^2\right) = k_B T_{c0} \left[\frac{1}{\delta} (t-1) |\psi|^2 + \frac{0.106}{\delta} |\psi|^4 \right]$$

Here $T_{c0} = T_c(H \to 0)$, $t = T/T_{c0}$, and $\delta = [N(0) v k_B T_{c0}]^{-1}$ (with $N(0)$- the electronic density of states per unit volume at the Fermi energy, and v- the volume of the small SC particle), is the quantum size parameter of the SC grain. The corresponding MF free energy is $\widetilde{f}_{GL}^{(0)}(T, H \to 0) = -\left(\frac{9.4}{2\delta}\right) k_B T_{c0} (1-t)^2$.

For the isolated SC layer at high magnetic field and low temperature $T \ll T_c(H \to 0)$ it was found that [7], $\alpha = \frac{1}{4\hbar\omega_c} \ln\left(\frac{H_{c2}}{H}\right) \approx \frac{1}{4\hbar\omega_c}(1-h)$, with $h \equiv H/H_{c2}(T \to 0)$, and $\beta \approx \frac{1.38}{(\hbar\omega_c)^2 E_F}$. Here $\omega_c = eH/m^* c$ is the cyclotron frequency, with m^* the in-plane effective cyclotron mass, and E_F the Fermi energy. The corresponding MF free energy is $\widetilde{f}_{GL}^{(0)}(T \to 0, H) \approx -\left(\frac{1}{16\beta_a}\right) E_F (1-h)^2$. For general T , and H values near the MF transition line, $H_{c2}(T) = \frac{\phi_0}{2\pi\xi(T)^2} = H_{c2}(0)(1 - T/T_{c0})$, the corresponding MF free energy has the well known form $\widetilde{f}_{GL}^{(0)}(T,H) = \widetilde{f}_{GL}^{(0)}(0,0)(1-t-h)^2 = \widetilde{f}_{GL}^{(0)}(0,0)(1-T/T_{c0})^2 [1 - H/H_{c2}(T)]^2$, so that by equating the coefficient $\widetilde{f}_{GL}^{(0)}(0,0)$ in the two limiting regions of the phase boundary, i.e. $\widetilde{f}_{GL}^{(0)}(0,0) = \left(\frac{9.4}{2\delta}\right) k_B T_{c0} = \left(\frac{1}{16\beta_a}\right) E_F$, one finds: $\delta = \frac{k_B T_{c0}}{1.3 \times 10^{-2} E_F}$ with $\beta_a \approx 1$.

Using the well known BCS expression for the zero temperature coherence length, $\xi(0) = 0.18\hbar v_F / k_B T_{c0}$, we find that

$$\delta \approx 28 \left(\frac{1}{k_F \xi(0)} \right) \tag{9}$$

This enables us to estimate the effective spatial size of the SC grain in the zero field limit. Since our original model system consists of a 2D SC layer, the volume $v \equiv a^2$ is a 2D area, and the DOS function is that of a 2D electron gas, $N(0) = m^*/2\pi\hbar^2 = \frac{k_F^2}{4\pi}\frac{1}{E_F}$, so that $\delta \approx 35\left(\frac{\xi(0)}{a}\right)\left(\frac{1}{k_F a}\right)$. Comparing this expression to Eq.(9) , we find that the radius of the effective SC grain $a \sim \xi(0)$, which is approximately equal to $a_{H_{c2}(0)}$- the smallest length scale in a 2D SC condensate in a magnetic field $H \approx H_{c2}(0)$. For MgB_2 we have: $T_{c0} \approx 40K$, $E_F \approx 12500K$, so that $\delta = 0.23$.

These results show that a single SC layer in a high magnetic field above the vortex lattice melting point is equivalent to a 0D superconductor at zero magnetic field [8]. The coupled layer model is therefore equivalent to a 1D Josephson array of small SC grains, discussed, e.g. in [8], or in [16]. For the relatively large effective quantum size parameter $\delta = 0.23$, estimated above, the numerical simulations reported in Ref.[8] show that the reduction of the transition width by the interlayer coupling is not very significant.

To make this feature useful in our analysis of experimental data we have approximated our result by means of an interpolation function, suggested by Ito et al.[5] to fit their experimental dHvA data for a quasi 2D organic superconductor, namely:

$$\Phi_{0,interp}(x;\kappa) = x + \sqrt{\nu_\kappa^2 + x^2} \tag{10}$$

where the fitting parameter ν_κ depends only on the interlayer coupling. The equivalence of Eq.(10) to the interpolation formula presented in Ref.[5] is made clear if we note from Eq.(5) that $x = \frac{\alpha}{2\beta\beta_a\alpha_{0I}} = \frac{\Delta_0^2}{2\alpha_{I0}}\left(1 - \frac{H}{H_{c2}(T)}\right)$, where Δ_0 is the SC gap parameter at $T = 0$, and $H = 0$.

The best fitting function $\Phi_{0,interp}(x;\kappa)$ is represented in Fig. (1) by the dashed lines for the limiting cases $\kappa = 0$ and $\kappa \to \infty$. At zero coupling the parameter ν_κ can be obtained by comparing $\Phi_{0,interp}(x;0)$ with $\Phi_0(x;0) = 2\left(x + \exp(-x^2)/\sqrt{\pi}\,\mathrm{erfc}\,(-x)\right)$, to yield $\nu_{\kappa=0} = 2/\sqrt{\pi} \approx 1.13$. In the strong coupling limit the best fit is obtained for $\nu_{\kappa=100} = .51$. Thus, the entire range of the actual smearing parameter $\alpha_I = \nu_\kappa\alpha_{0I}$ is obtained with $\nu_\kappa = .51 - 1.13$.

The parameter $\alpha_I = \nu_\kappa\sqrt{\frac{k_BT}{2\beta\beta_a}}$, which controls the smearing of the phase transition by the fluctuations, is related to the parameter α_F introduced in Ref. [6] (denoted there by α) by: $\alpha_F = 2\alpha_I/\Delta_0^2$, where Δ_0 can be identified with Δ_E of Ref. [6]. Using the above value of β, obtained from the 2D electron gas model, we find that:

$$\alpha_I \approx 0.35\nu_\kappa\hbar\omega_c\sqrt{E_Fk_BT} \tag{11}$$

which reflects the smearing effect due to the magnetic field, the suppression of this smearing by the interlayer coupling parameter κ, and the thermal smearing effect.

For the parameters characterizing the MgB_2 data, reported by Fletcher et al. [6], i.e. with $m^* \approx 0.3m_e$, $T = 0.32K$, $\Delta_0 = 200K$, $F = 2930T$, so that $E_F = \hbar\omega_cF/H = 12464K$, our theoretical estimate is $\alpha_I \approx 479K^2$, or $\alpha_F \approx 0.024$. This result is similar to, but somewhat smaller than the best fitting value of α_F obtained in Ref.[6].

This is quite a reasonable result since, as noted above, one should regard the calculated width as a lower bound on the smearing of the SC phase transition by all types of thermal fluctuations of the SC order parameter. Furthermore, as clearly seen in Fig.(1), the deviation of the fluctuation effect predicted in our 3D model from the best fit to the experimentally observed data is rather small in the magnetic field region bellow MF H_{c2}, and becomes more significant at fields well above the MF transition. This behavior is reasonably explained by the omission of many fluctuation degrees of freedom in our vortex chain model [13], which is expected to weaken progressively the fluctuation effect with respect to the actually observed one as the magnetic field increases above MF H_{c2}.

It should be also emphasized that the smearing parameter α_I, given in Eq.(11), is independent of the SC gap parameter Δ_0, an important parameter determining the damping of the dHvA oscillations in the SC state [7]. In the fitting procedure employed in Ref.[6] Δ_0 was found to disagree with the SC gap parameter Δ_π derived by other methods. Our estimate of the SC fluctuations effect from the damping of the dHvA oscillation in the SC state is thus unaffected by such a disagreement.

In conclusion, it was shown here that the transition to the low temperature SC state in a pure, extremely type-II, 3D superconductor is smeared dramatically by the magnetic field, comparable in magnitude to the broadening of the transition observed in quasi 2D superconductors. The dimensionality reduction by the magnetic field, responsible for this smearing, is shown to take place in a broad field range above the vortex lattice melting point, where the system of SC fluctuations is equivalent to a 1D array of SC quantum dots. The theoretically predicted width of the transition region is found to be in good agreement with experimental data of the dHvA effect in the SC state of MgB_2.

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